Dynamic Simulation of a Crude Oil Unit

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Abstract

This paper presents a dynamic model for the crude oil distillation unit. After years of experiments, our model is a compromise between a good results accuracy requiring a complex model and its reasonable dimensions. Because we used DIVA simulator that is "block oriented", the models representing the main column, sidestripers, pumparounds and condenser with the tank, describe the plant; the whole unit is represented by these connected elements. At the final of this work we present some simulation results.

Keywords: crude oil unit, dynamic model, simulation.

1. Introduction

The crude oil unit, as a part of the Atmospheric and Vacuum Distillation unit, is one of the most important plants in a refinery. Due to its own place (its products being feeds for other important units) and complexity, it is very important to have a powerful instrument to study intimately this multi-component distillation process.

Thus, a software simulator focused on the process dynamics can be one of these analyzing tools; furthermore it can be used not only for research purposes, but also as a support for plant operators training, giving a good way for safe "experiments" of various operating strategies.

There is an alternative: to use an "industrial", "factory made" simulator covering a large class of applications or to build-up a personal one, focused only on the problems regarding the crude oil unit. Obviously, for research purposes, which need a very close "look inside the process", a dedicated tool is required, having different features from the general simulators. This way, using an appropriate model, the user is able to know the basics of the distillation process and even to improve the model itself – something impossible in the case of the "industrial" simulators that offer some standard, inflexible models and nothing more.

In order to have the benefits of a dedicated simulator it is necessary to build-up a mathematical model for the process, then to find an appropriate method to integrate it and finally to display the simulation results in an accessible form for the user.

After years of experiments in this field, the authors present in this paper a model for the crude oil distillation unit and suggest a modern solution to integrate it and display/analyze the simulation results.

2. The mathematical model for the crude oil unit dynamics

It is quite difficult to build-up a dynamic model for the multi-component distillation due to the process complexity and the problems which may affect the numerical integration of the model equations even using "top level" algorithms and powerful digital equipments.

We propose a model representing a compromise between good results accuracy and a reasonable model dimension in order to require a non-prohibitive execution time for the integration routine. Based on our own experience and literature study too, we have some simplifying assumptions:

- Perfectly mixed component on column stages;
- Equilibrium (theoretical) stages;
- Negligible vapor holdups;
- Constant pressure profile;
- Total condenser with "perfect" controlled temperature.

As shown in figure 1, the crude oil unit consists in one main column with two pumparounds and four sidedraws to the sidestripers; the top vapor is totally condensed and stored in a tank where the water is decanted; a part of the top product turns back into the column as external reflux.

The model for the entire unit is obtained from the models for each particular element of the plant as shown as follows.

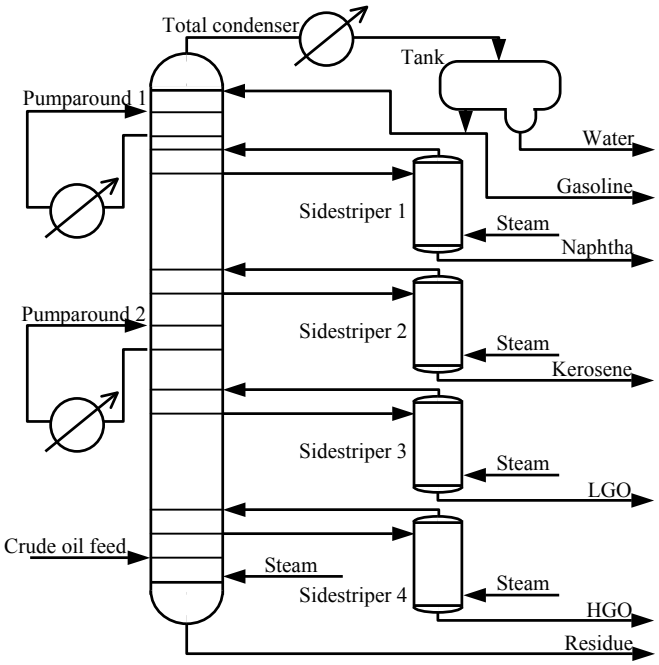

Fig.1. The crude oil distillation unit.

The columns and sidestripers

The model for the main column and the sidestripers is the same, the only thing that differs being the number of trays (considered as a "structural parameter" for the model). It is mainly based on equations for total material balance, component material balance, energy balance and liquid-vapor equilibrium:

► *Column top (k = 1), see figure 2a:*

$$m_1 \dot{X}_{1,i} = FL_1 \cdot XFL_{1,i} + FV_1 \cdot YFV_{1,i} + \\ + V_2 \cdot K_{2,i} \cdot X_{2,i} - VE_1 \cdot K_{1,i} \cdot X_{1,i} - \\ - X_{1,i} \cdot (FL_1 + FV_1 + V_2 - VE_1) \quad i = \overline{1, NC-1} \tag{1}$$

$$0 = 1 - \sum_{i=1}^{NC} X_{1,i} \tag{2}$$

$$0 = Y_{1,i} - K_{1,i} \cdot X_{1,i} \quad i = \overline{1, NC} \tag{3}$$

$$0 = 1 - \sum_{i=1}^{NC} Y_{1,i} \tag{4}$$

$$\tfrac{2}{3}\, bm_1 \cdot LE_1^{\left(-\frac{1}{3}\right)} \cdot \dot{LE}_1 = FL_1 + FV_1 + V_2 - VE_1 - LE_1 \tag{5}$$

$$0 = FL_1 \cdot HFL_1 + FV_1 \cdot HFV_1 + V_2 \cdot HV_2 - VE_1 \cdot HV_1 - HL_1 \cdot (FL_1 + FV_1 + V_2 - VE_1) - \sum_{i=1}^{NC} HLP_{1,i} \cdot \dot{X}_{1,i} \tag{6}$$

$$0 = m_1 - bm_1 \cdot LE_1^{\frac{2}{3}} - m_{0,1} \tag{7}$$

$$0 = LE_1 - L_1 - DL_1 \tag{8}$$

$$0 = VE_1 - V_1 - DV_1 \tag{9}$$

► <u>*Tray k*</u> *(k = 2...NS – 1), see figure 2b:*

$$m_k \dot{X}_{k,i} = FL_k \cdot XFL_{k,i} + FV_k \cdot YFV_{k,i} + L_{k-1} \cdot X_{k-1,i} + V_{k+1} \cdot K_{k+1,i} \cdot X_{k+1,i} - VE_k \cdot K_{k,i} \cdot X_{k,i} - X_{k,i} \cdot (FL_k + FV_k + L_{k-1} + V_{k+1} - VE_k) \quad i = \overline{1, NC-1} \tag{10}$$

$$0 = 1 - \sum_{i=1}^{NC} X_{k,i} \tag{11}$$

$$0 = Y_{k,i} - K_{k,i} \cdot X_{k,i} \quad i = \overline{1, NC} \tag{12}$$

$$0 = 1 - \sum_{i=1}^{NC} Y_{k,i} \tag{13}$$

$$\tfrac{2}{3}\, bm_k \cdot LE_k^{\left(-\frac{1}{3}\right)} \cdot \dot{LE}_k = FL_k + FV_k + L_{k-1} + V_{k+1} - VE_k - LE_k \tag{14}$$

$$0 = FL_k \cdot HFL_k + FV_k \cdot HFV_k + L_{k-1} \cdot HL_{k-1} + V_{k+1} \cdot HV_{k+1} - VE_k \cdot HV_k - HL_k \cdot (FL_k + FV_k + L_{k-1} + V_{k+1} - VE_k) - \sum_{i=1}^{NC} HLP_{k,i} \cdot \dot{X}_{k,i} \tag{15}$$

$$0 = m_k - bm_k \cdot LE_k^{\frac{2}{3}} - m_{0,k} \tag{16}$$

$$0 = LE_k - L_k - DL_k \tag{17}$$

$$0 = VE_k - V_k - DV_k \tag{18}$$

► <u>*Column bottom*</u> *(k = NS), see figure 2c:*

$$m_{NS} \dot{X}_{NS,i} = FL_{NS} \cdot XFL_{NS,i} + FV_{NS} \cdot YFV_{NS,i} + L_{NS-1} \cdot X_{NS-1,i} - VE_{NS} \cdot K_{NS,i} \cdot X_{NS,i} - X_{NS,i} \cdot (FL_{NS} + FV_{NS} + L_{NS-1} - VE_{NS}) \quad i = \overline{1, NC-1} \tag{19}$$

$$0 = 1 - \sum_{i=1}^{NC} X_{NS,i} \tag{20}$$

$$0 = Y_{NS,i} - K_{NS,i} \cdot X_{NS,i} \quad i = \overline{1, NC} \tag{21}$$

$$0 = 1 - \sum_{i=1}^{NC} Y_{NS,i} \tag{22}$$

$$\dot{m}_{NS} = FL_{NS} + FV_{NS} + L_{NS-1} - VE_{NS} - LE_{NS} \tag{23}$$

$$0 = FL_{NS} \cdot HFL_{NS} + FV_{NS} \cdot HFV_{NS} + L_{NS-1} \cdot HL_{NS-1} - VE_{NS} \cdot HV_{NS} - HL_{NS} \cdot (FL_{NS} + FV_{NS} + L_{NS-1} - VE_{NS}) - \sum_{i=1}^{NC} HLP_{NS,i} \cdot \dot{X}_{NS,i} \tag{24}$$

$$0 = LE_{NS} - DL_{NS} \tag{25}$$

$$0 = LE_{NS} - L_{NS} - DL_{NS} \tag{26}$$

$$0 = VE_{NS} - V_{NS} - DV_{NS} \tag{27}$$

In these equations, the enthalpies and liquid-vapor equilibrium constant must be specified, for example by polynomial functions of temperature (the most simple case) or using some more complex and accurate correlations of pressure, temperature and composition, if enough information is available to the user (i.e. Chao-Seader, Boston-Britt a.s.o.) [4, 5, 6].

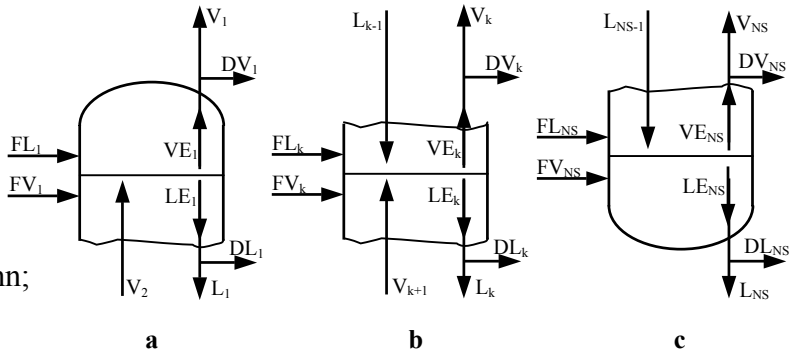

Fig. 2. Column streams
a- column top;
b- a tray inside the column;
c- column bottom.

We must emphasize a few characteristics of this model:

- The system is ill conditioned, stiff, imposing serious limitations for the integration step in order to have a stable numerical solution;
- The transient time has a value in the range of 5…25 hours (for industrial crude oil distillation units);
- The system dimension is very large and may lead to some memory management problems; thus we must operate some dimensional reductions (i.e. observing that only a few trays in the column have external feeds or sidedraws).

The pumparounds

The model for the pumparounds is mainly based on the equation for the heat transfer from the cooled product stream to the cooling agent, obviously without any changes in product composition and flow rate:

$$Mpa/_{FIN} \cdot \dot{T}OUT = = TIN - TOUT - Qpa/_{(FIN \cdot c_p)} \quad (28)$$

$$0 = XIN - XOUT \quad (29)$$

$$0 = FIN - FOUT \quad (30)$$

The condenser with tank

For this assembly we have adopted a very simple model, considering the case of a total condenser with "perfect" temperature control and constant liquid holdup in the tank. The decanted water accumulation is not modeled here, but it is included in the equations used for simulation:

$$0 = TCOND - TFIX \quad (31)$$

$$0 = XCOND_i - YIN_i \quad i = \overline{1, NC} \quad (32)$$

$$0 = FCOND - FVAP \quad (33)$$

3. A suggestion for the dynamic simulation of the entire distillation unit

To simulate the dynamics of the crude oil unit means in fact to integrate its mathematical model equations, requiring adequate routines for numerical integration and graphical representation of the simulation results. The authors of this paper suggest a very versatile and powerful software oriented on dynamic simulations for industrial plants, DIVA (Dynamische Simulation Verfahrenstechnischer Anlagen), developed at the Stuttgart University [1]. This simulator is running under Linux operating system and integrates some sets of high-level routines for solve/integrate complex algebraic and differential equation systems. It is not the place here to describe the features of DIVA simulator, but we want to emphasize that, being oriented on simulations over the industrial plants, it works with the concept of "block device": the entire plant is divided in relevant parts in accord with topologic and functional rules. Every block is described by its own model and external connections, giving a natural way to aggregate the entire

plant, a way we call "a structural approach".

There are some important advantages using this manner of work:

- A very easy to understand representation of the plant inside the simulator;
- An easier way to describe the plant through a mathematical model, using multiple simple models for the blocks instead of a single complex model for the entire plant;
- The user is able to test the parts of the plant and to identify mismatches in the models;
- A possibility to have an open structure that will permit anytime improvements and additional modules.

For detailed information about DIVA simulation environment that include the graphical representation feature (using a dedicated MATLAB toolbox) the reader may consult the references [1, 2, 3].

We tested our model on an industrial crude oil unit (its structure being shown in figure 1); some significant data are presented in table 1.

Table 1. Some data about the crude oil unit.

Number of trays in the main column	30
Number of trays in the sidestriper	3
Number of pseudo-components in the feed	37, including water
Feed type	pre-flashed
Feed flow rate	0.57 kmol/s
Reflux ratio	0.23
Molar holdup on column trays	3.0 kmol

Regarding the simulator settings, we used in DIVA the NLEQ1S solver (Newton method with variable damping strategy) to get the initial conditions and LIMEXS integrator (extrapolation method with variable step size).

In this paper it is not the place to analyze the simulation results (it will be the topic of a future work), but just as example we present the following diagrams.

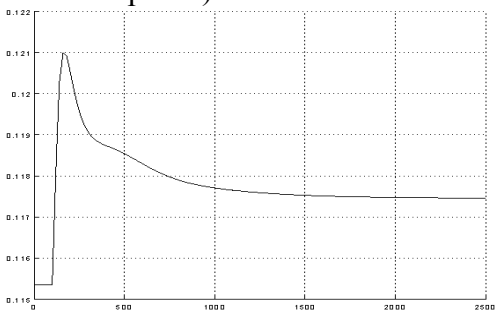

Fig. 3.Comp. 5 in top product (gasoline) when steam flow rate increases.

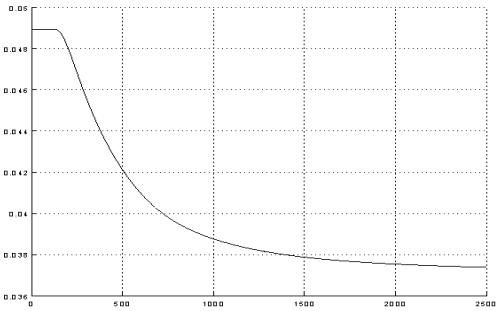

Fig. 4. Comp. 5 in bottom of sidestriper 1 (naphtha) when steam flow rate increases.

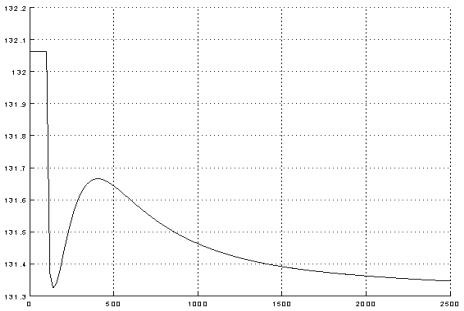

Fig. 5. Temperature on tray 1 when reflux ratio increases.

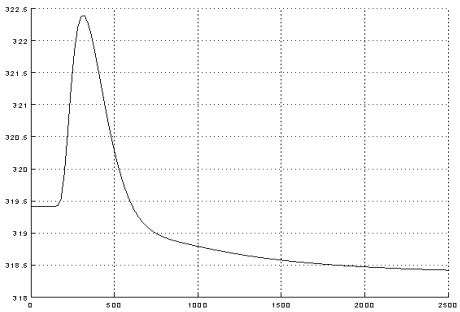

Fig. 6. Temperature on tray 30 when reflux ratio increases.

4. Conclusions

In this paper was presented a dynamic model for the crude oil distillation unit. The model for the whole plant consists in the models for a few blocks representing elements of the plant: the main column, sidestripers, pumparounds and condenser with the tank. This partition of the unit in sub-components is very useful for an easy model implementation and integration in DIVA, the software simulator we used to simulate the crude oil plant. At the final of our work we present some simulation results.

Nomenclature

Molar flow rates:

FL – liquid feed on tray;
FV – vapor feed on tray;
LE – liquid leaving the tray;
VE – vapor leaving the tray;
DL – liquid sidedraw from tray;
DV – vapor sidedraw from tray;
L – liquid remaining after sidedraw;
V – vapor remaining after sidedraw;
FIN – product to heat exchanger;
FOUT – product from heat exchanger;
FVAP – vapor to condenser;
FCOND – condensed liquid.

Molar fractions:

XFL – pseudo-component in liquid feed;
YFV – pseudo-component in vapor feed;
X – pseudo-component in liquid on tray;
Y – pseudo-component in vapor on tray;
XIN – pseudo-component in product to heat exchanger;
XOUT – pseudo-component in product from heat exchanger;
YIN – pseudo-component in vapor to condenser;
XCOND – pseudo-component in condensed liquid.

Temperatures:

TIN – product to heat exchanger;
TOUT – product from heat exchanger;
TFIX – setpoint for condensed liquid;
TCOND – condensed liquid.

Molar enthalpies:

HFL – liquid feed;
HFV – vapor feed;
HL – liquid on tray;
HV – vapor on tray;
HLP – pseudo-component in liquid phase.

Others:

K – liquid-vapor constant;
m_0 – constant liquid holdup on tray;
m – liquid holdup on tray;
bm – coefficient in the holdup equation;
NS – number of column trays;
Mpa – product holdup in the heat exchanger;
Qpa – heat exchange on pumparound;
cp – product specific heat.

Indexes:

i – pseudo-component;
k – tray number.

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